

# A Semi-Analytical Propagation Equation Model for the Study of Signal Propagation in Kerr Nonlinear Nanophotonic Waveguides

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**Abstract:** A nonlinear propagation equation model is derived in the case of periodic nanophotonic waveguides using reciprocity relations. The frequency dependence of the Self Phase Modulation (SPM) coefficient is analyzed and higher order nonlinear terms are calculated in the middle and the edge of the guided band.

## Introduction

Nanophotonic structures are constantly attracting increased attention for the realization of future optical integrated circuits with increased scale of integration. Particular attention is given to artificial periodic dielectric structures usually referred to as Photonic Crystals (PC) [1]. PCs can exhibit photonic bandgaps, i.e. a range of frequencies where no guided mode exists. By introducing defects in a PC structure, one can form waveguides and cavities in which light is tightly confined. PC waveguides provide an efficient means of guiding light by allowing the realization of sharp optical bends. As in the case of optical fibers, signal processing could be accomplished in the nonlinear regime [2]. In another context, a large chain of coupled cavities can be thought of as a novel type of waveguide where light propagates through evanescent wave coupling from cavity to cavity. This new type of waveguide is called the Coupled Resonator Optical Waveguide (CROW) [3] and has many interesting properties. By appropriately positioning the resonators, it is possible to construct sharp, lossless and reflection-less bends throughout the entire CROW band. Another important property of the CROW is its ability to drastically slow down the optical wave (the slow light concept) which can find important applications in the realization of compact optical delay lines. The low group velocity and large optical field amplitudes of the localized modes lead to an enhancement of nonlinear effects which could potentially be useful for signal processing.

In this paper, we derive a propagation equation model to describe the pulse propagation inside a single mode nonlinear periodic nanophotonic waveguide which is very similar to the one used in conventional constant cross-section optical waveguides [4]. The derivation is based on a straight forward application of the reciprocity relations [5] in Maxwell's equations. The model provides an efficient means of simulating nonlinear behaviour while avoiding the computational complexity of more complex Finite Difference Time Domain (FDTD) method [6].

## Envelope Functions of the Guided Mode

Assuming a single mode waveguide, the electric field  $\mathbf{E}$  can be expressed as

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_p(\mathbf{r}, t) + c.c. \quad (1)$$

where

$$\mathbf{E}_p(\mathbf{r}, t) = \int_P d\omega a(z, \omega) \mathbf{E}_\omega e^{-j\omega t} \quad (2)$$

where the spectrum of  $\mathbf{E}_p$  has a bandwidth of  $\delta\omega$  and lies near a central frequency  $\omega = \omega_0$  and  $P = [\omega_0 - \frac{1}{2}\delta\omega, \omega_0 + \frac{1}{2}\delta\omega]$ . The envelope functions  $A(z, t)$  of the mode can be defined as

$$A(z, t) = \int_P d\omega a(z, \omega) e^{j\Delta\beta z - j\Delta\omega t} \quad (3)$$

where  $\Delta\omega = \omega - \omega_0$ . Using Bloch's theorem, the mode of the waveguide is written as

$$\mathbf{E}_\omega = \mathbf{e}_\omega e^{j\beta(\omega)z} \quad (4)$$

where  $\mathbf{e}_\omega$  is the periodic vector function and  $\beta(\omega)$  is the propagation constant of the mode. The guided mode obeys

$$\nabla \times \mathbf{H}_\omega = -j\omega \varepsilon_L \mathbf{E}_\omega, \quad \nabla \times \mathbf{E}_\omega = j\omega \mu \mathbf{H}_\omega \quad (5)$$

and the mode is normalized so that:

$$N = \int_S dS (\mathbf{E}_\omega \times \mathbf{H}_\omega^* + \mathbf{H}_\omega \times \mathbf{E}_\omega^*) \cdot \mathbf{z} = 1 \quad (6)$$

where  $\varepsilon_L$  is the linear part of the dielectric constant. Fig. 1 illustrates the dispersion relation of the guided mode of a CROW based on 2D photonic crystal defect cavities (see figure inset) calculated using the Plane Wave Expansion (PWE) method [7]. In this case the electric field is polarized along the y direction, i.e.  $\mathbf{e}_{1,\omega} = \mathbf{y}e_y(x, z)$ . The refractive index of the rods was taken  $n_a = 3.4$  while that of the surrounding medium was taken  $n_b = 1.0$ . The PC lattice constant is taken  $a = 0.6 \mu\text{m}$  while the adjacent cavity spacing  $D$  and the rod radius  $r_a$  are  $D = 2a$  and  $r_a = 0.18a$  respectively. The guided mode band extends from 185.7THz to 204.8THz. Also shown in the same figure is the slow down factor  $S$  of the mode defined as  $S = c/v_g$ , where  $c$  is the speed of light in vacuum, while  $v_g$  is the group velocity of the mode. Near the band edges,  $S$  is large, implying larger

amplitudes for the modal fields and hence an enhancement of nonlinear effects. This is illustrated in Fig. 2 (a) and (b), where the normalized modal fields  $e_y(x,z)$  are plotted assuming  $\beta=\pi/2D$  (middle of the band) and  $\beta=0.05\pi/D$  (near the band edge) respectively and it is deduced that the modal amplitude is stronger in the latter case. Fig. 2 illustrates the modal field distribution at  $\beta=0.25\pi/D$  (middle of the guided band) and  $\beta=0.05\pi/D$  (band edge). It is deduced that although the shape of the main lobe of the mode does not change drastically, the modal amplitudes are significantly enhanced.

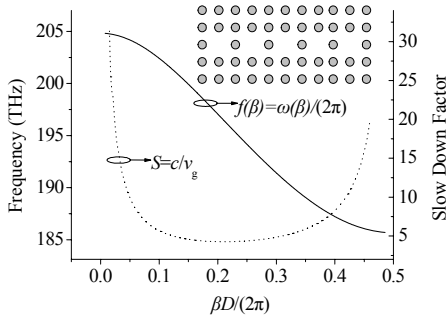


Fig. 1: The dispersion relation and slow down factor  $S$  of the guided mode of a coupled resonator optical waveguide (CROW) formed out of 2D photonic crystal defect cavities spaced  $D=2a$  apart

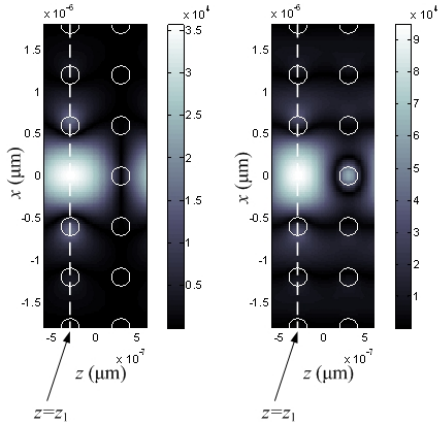


Fig. 2: a) and b) the modal field distribution of the electric field  $e_y$  of the modes inside the waveguide cell at  $\beta=\pi/D/2$  and  $\beta=0.05\pi/D/2$ .

Expanding the modal field and the propagation constant around  $\omega=\omega_0$ ,

$$\mathbf{e}_\omega = \sum_{n=0}^{\infty} \frac{\partial^n \mathbf{e}_{\omega_0}}{\partial \omega^n} \frac{\Delta \omega^n}{n!}, \quad \beta(\omega) = \sum_{n=0}^{\infty} \beta_n \frac{\Delta \omega^n}{n!} \quad (7)$$

with  $\beta_n = \partial^n \beta(\omega_0) / \partial \omega^n$ . Substituting (7) in (2) and using (3), one obtains:

$$\begin{aligned} \mathbf{E}(\mathbf{r}, t) &= \sum_{n=0}^{\infty} \frac{\partial^n A(z, t)}{\partial t^n} \frac{\partial^n \mathbf{e}_{\omega_0}}{\partial \omega^n} \frac{j^n}{n!} e^{j\beta_0 z - j\omega_0 t} + c.c. \\ &\cong A(z, t) \mathbf{e}_{\omega_0} e^{j\beta_0 z - j\omega_0 t} + c.c. \end{aligned} \quad (8)$$

where the second approximate equality is obtained by keeping only the first order terms. According to

equation (8) the electric field is approximately written in terms of the Bloch function at  $\omega=\omega_0$ , modulated by the envelope function  $A(z, t)$ . Differentiating with respect to  $z$

$$\frac{\partial A(z, t)}{\partial z} = \int_P d\omega \left[ \frac{\partial a}{\partial z} + j\Delta\beta a \right] e^{j\Delta\beta z - j\Delta\omega t} \quad (9)$$

where  $\Delta\beta = \beta(\omega) - \beta(\omega_0)$ . Expanding  $\Delta\beta$  around  $\omega=\omega_0$ , equation (9) is written as

$$\frac{\partial A(z, t)}{\partial z} = \int_P d\omega \frac{\partial a}{\partial z} e^{j\Delta\beta z - j\Delta\omega t} + \sum_{n=1}^{\infty} \frac{j^{n+1} \beta_n}{n!} \frac{\partial^n A}{\partial t^n} \quad (10)$$

Equation (10) provides an evolution equation for the envelope function of the mode. In the next section the integral in the right hand side will be expressed in terms of the nonlinear contribution using the reciprocity relations.

### Application of Reciprocity Relations

The total electromagnetic field ( $\mathbf{E}, \mathbf{H}$ ) obeys the usual time dependent Maxwell's equations:

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}, \quad \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} \quad (11)$$

where  $\varepsilon = \varepsilon_L + \varepsilon_{NL} |\mathbf{E}|^2$  is the nonlinear dielectric constant of the waveguide. Setting  $\mathbf{F} = \mathbf{E} \times \mathbf{H}_{\omega_0}^* + \mathbf{E}_{\omega_0}^* \times \mathbf{H}$  and applying Green's theorem one obtains:

$$\begin{aligned} \frac{\partial}{\partial z} \int_S \mathbf{F} \cdot \mathbf{z} dS &= - \int_S \left( \mu \mathbf{H}_{\omega_0}^* \cdot \frac{\partial \mathbf{H}}{\partial t} + \varepsilon \mathbf{E}_{\omega_0}^* \cdot \frac{\partial \mathbf{E}}{\partial t} \right) dS \\ &\quad - j\omega_1 \int_S \left( \varepsilon_L \mathbf{E} \cdot \mathbf{E}_{\omega_0}^* + \mu \mathbf{H} \cdot \mathbf{H}_{\omega_0}^* \right) dS \end{aligned} \quad (12)$$

where  $S$  is any plane perpendicular to the propagation direction  $z$ . Using this equation, one obtains:

$$\frac{\partial}{\partial z} \int d\omega a R(\omega) e^{-j\omega t} = j \int d\omega a M(\omega) e^{-j\omega t} \quad (13)$$

with

$$R(\omega) = \int_S dS \left( \mathbf{E}_\omega \times \mathbf{H}_{\omega_0}^* + \mathbf{E}_{\omega_0}^* \times \mathbf{H}_\omega \right) \cdot \mathbf{z} \quad (14)$$

$$M(\omega) = \int_S dS \left\{ \mu \Delta\omega \mathbf{H}_\omega \cdot \mathbf{H}_{\omega_0}^* + (\omega \varepsilon - \omega_0 \varepsilon_L) \mathbf{E}_\omega \cdot \mathbf{E}_{\omega_0}^* \right\} \quad (15)$$

Setting  $\mathbf{F}_1 = \mathbf{E}_\omega \times \mathbf{H}_{\omega_0}^* + \mathbf{E}_{\omega_0}^* \times \mathbf{H}_\omega$  and applying Green's divergence theorem, one obtains

$$\frac{\partial R}{\partial z} = j\Delta\omega \int_S \left[ \mu \mathbf{H}_{\omega_0}^* \cdot \mathbf{H}_\omega + \varepsilon_L \mathbf{E}_{\omega_0}^* \cdot \mathbf{E}_\omega \right] dS \quad (16)$$

Combining (16) and (13), the following equation is obtained:

$$\int d\omega \frac{\partial a}{\partial z} R(\omega) e^{j\Delta\beta z} e^{-j\omega t} = G(t) \quad (17)$$

where the function  $G(t)$  is

$$G(t) = j \int d\omega \omega a(z, \omega) e^{-j\omega t} \int_S dS \varepsilon_{NL} |\mathbf{E}|^2 \mathbf{e}_\omega \cdot \mathbf{e}_{\omega_0}^* \quad (18)$$

Inverting the Fourier transform in (17) and re-integrating in  $P$ , equation (17) is written as

$$\int_P d\omega \frac{\partial a}{\partial z} e^{j\Delta\beta z} e^{-j\Delta\omega t} = \int_P \tilde{G}(\omega) R^{-1}(\omega) e^{-j\Delta\omega t} \quad (19)$$

where Expanding  $R^{-1}$  around  $\omega = \omega_0$ , one obtains:

$$R^{-1}(\omega) = \sum_{r=0}^{\infty} R_n \frac{(\Delta\omega)^n}{n!} \quad (20)$$

and using (20) in (19) along with (10), one obtains the following expression:

$$\frac{\partial A}{\partial z} = \sum_{r=0}^{\infty} \frac{j^r}{r!} R_r \frac{\partial^r G_p}{\partial t^r} + \sum_{n=1}^{\infty} \frac{j^{n+1}}{n!} \beta_n \frac{\partial^n A}{\partial t^n} \quad (21)$$

where  $\tilde{G}(\omega)$  is the spectrum of  $G(t)$

$$G_p(t) = j \int_P d\omega \omega a e^{-j\Delta\omega t} \int_S dS \varepsilon_{NL} |\mathbf{E}|^2 \mathbf{e}_\omega \cdot \mathbf{e}_{\omega_0}^* \quad (22)$$

In the next section  $G_p(t)$  will be expressed in terms of the envelope function  $A$  in order to complete the derivation.

### Nonlinear Perturbation

To express  $G_p(t)$  in terms of the envelope function of the guided mode, one makes use of the fact that

$$|\mathbf{E}|^2 = \mathbf{E} \cdot \mathbf{E} \cong 2|\mathbf{E}_p|^2 \quad (23)$$

In (23), the terms oscillating around  $\pm 2\omega_0$  are ignored. Using (2)

$$|\mathbf{E}|^2 \cong 2|\mathbf{E}_p|^2 = 2 \int_P d\omega_1 a(z, \omega_1) \int_P d\omega_2 a^*(z, \omega_2) \times e^{j\Delta\beta_p z - j\Delta\omega_1 t - j\Delta\beta_q z + j\Delta\omega_2 t} \mathbf{e}_{\omega_1} \cdot \mathbf{e}_{\omega_2}^* \quad (24)$$

Defining the function

$$T = 2\omega \int_S dS \varepsilon_{NL} (\mathbf{e}_{\omega_1} \cdot \mathbf{e}_{\omega_2}^*) (\mathbf{e}_\omega \cdot \mathbf{e}_{\omega_0}^*) \quad (25)$$

and expanding around  $\omega_1 = \omega_2 = \omega = \omega_0$ ,

$$T = \sum_{\mu\nu\kappa} T_{\mu\nu\kappa} \frac{(\Delta\omega)^\mu (\Delta\omega_1)^\nu (\Delta\omega_2)^\kappa}{\mu! \nu! \kappa!} \quad (26)$$

and using (26) and (24) in (22), the nonlinear perturbation is written as:

$$Q_p = j \sum_{\mu\nu\kappa} \frac{j^{\mu+\nu-\kappa}}{\mu! \nu! \kappa!} T_{\mu\nu\kappa} \frac{\partial^\mu A}{\partial t^\mu} \frac{\partial^\kappa A^*}{\partial t^\kappa} \frac{\partial^\nu A}{\partial t^\nu} \quad (27)$$

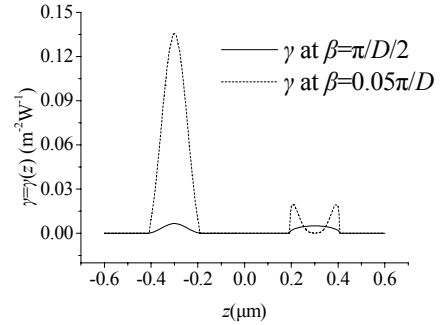


Fig. 3: The SPM coefficient for the CROW of Fig. 1 at the middle and the edge of the guided band.

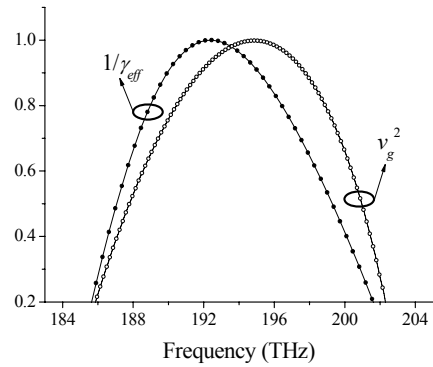


Fig. 4: Frequency dependence of  $1/\gamma_{eff}$  and  $v_g^2$

### Propagation Equation

Using (27) and (21), one obtains the following propagation equation for the envelope function:

$$\frac{\partial A(z, t)}{\partial z} = \sum_{n=1}^{\infty} \frac{j^{n+1}}{n!} \beta_n \frac{\partial^n A(z, t)}{\partial t^n} + \sum_{r=0}^{\infty} \frac{j^{r+\mu+\nu-\kappa+1}}{r! \mu! \nu! \kappa!} U_r \frac{\partial^r}{\partial t^r} \left[ T_{\mu\nu\kappa} \frac{\partial^\mu A}{\partial t^\mu} \frac{\partial^\kappa A^*}{\partial t^\kappa} \frac{\partial^\nu A}{\partial t^\nu} \right] \quad (28)$$

Keeping the nonlinear terms up to first order:

$$\frac{\partial A}{\partial z} = \sum_n \frac{j^{n+1} \beta_n}{n!} \frac{\partial^n A}{\partial t^n} + j\gamma |A|^2 A + \delta_1 \frac{\partial}{\partial t} (|A|^2 A) - (\delta_2 + \delta_3) |A|^2 \frac{\partial A}{\partial t} + \delta_4 A^2 \frac{\partial A^*}{\partial t} \quad (29)$$

where

$$\gamma = R_0 T_{000} = 2\omega_0 \int_S dS \varepsilon_{NL} |\mathbf{e}_{\omega_0}|^4 \quad (30)$$

is the SPM coefficient. Fig. 3 illustrates the value of  $\gamma$  across the unit cell of the CROW considered in Fig. 1, in the case where  $\beta = 1/2\pi/D$  (middle of the band) and  $\beta = 0.05\pi/D$  (near the band edge). The nonlinear refractive index of the rods was taken  $n_2 = 1.5 \times 10^{-17} \text{ m}^2/\text{W}$ . Note that unlike conventional waveguides, the SPM coefficient is periodic and

varies along the propagation direction. Also, as explained before, near the band edge, the modal fields  $\mathbf{e}_\omega$  are enhanced and hence the value of  $\gamma$  increases accordingly. The frequency dependence of the SPM coefficient is depicted in Fig. 5, where the normalized inverse of the effective SPM coefficient  $\gamma_{eff}$  is plotted and

$$\gamma_{eff} = \frac{1}{D} \int_{-D/2}^{D/2} \gamma(z) dz = \frac{2\omega_0}{D} \int_V dV \varepsilon_{NL} |\mathbf{e}_{\omega_0}|^4 \quad (31)$$

Also plotted in the figure is the normalized  $v_g^2$ . Comparing the two curves it is deduced that the SPM coefficient roughly exhibits a  $1/v_g^2$  behavior.

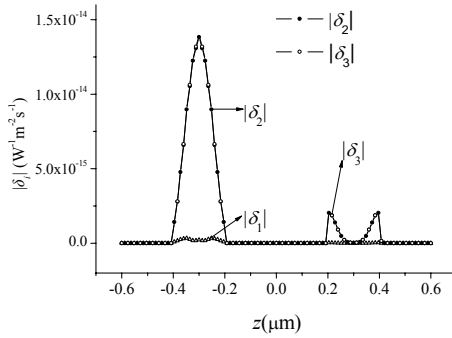


Fig. 5: Higher order nonlinear term coefficients for the CROW of Fig. 1 at  $\beta = \pi/D/2$

The nonlinear term with coefficient  $\delta_1$  corresponds to  $r=1$  and  $\mu=\nu=\kappa=0$  in (28) and is given by

$$\delta_1 = -U_1 T_{000} = u_1 \gamma \quad (32)$$

where  $U_1 = \partial(u^{-1})/\partial\omega = -u_1/u_0^2 = -u_1$  and

$$u_1 = \int_S dS \left( \frac{\partial \mathbf{e}_{\omega_0}}{\partial \omega} \times \mathbf{h}_{\omega_0}^* + \mathbf{e}_{\omega_0}^* \times \frac{\partial \mathbf{h}_{\omega_0}}{\partial \omega} \right) \cdot \mathbf{z} \quad (33)$$

The term  $\delta_2$  is obtained for  $\nu=1$  and  $r=\nu=\kappa=0$  in which case,

$$\delta_3 = 2\omega_0 \int_S dS \varepsilon_{NL} |\mathbf{e}_{\omega_0}|^2 \left( \frac{\partial \mathbf{e}_\omega}{\partial \omega} \cdot \mathbf{e}_{\omega_0}^* \right) \quad (34)$$

The term  $\delta_3$  corresponds to  $\mu=1$  and  $r=\nu=\kappa=0$  and is given by

$$\delta_2 = 2 \int_S dS \varepsilon_{NL} |\mathbf{e}_{\omega_0}|^2 \frac{\partial}{\partial \omega} (\omega \mathbf{e}_\omega \cdot \mathbf{e}_{\omega_0}^*) = \frac{\gamma}{\omega_0} + \delta_3 \quad (35)$$

The last nonlinear term is obtained for  $\kappa=1$  and  $r=\nu=\mu=0$  and is written as

$$\delta_4 = 2\omega_0 \int_S dS \varepsilon_{NL} |\mathbf{e}_{\omega_0}|^2 \left( \frac{\partial \mathbf{e}_\omega}{\partial \omega} \cdot \mathbf{e}_{\omega_0} \right) = \delta_3^* \quad (36)$$

Inspecting equations (32)-(36), one deduces that, as expected the higher order nonlinear contributions arise from the frequency dependence of the Bloch function  $\mathbf{e}_\omega$ .

In Fig. 5, the value of the higher order nonlinear coefficients at the middle of the CROW band ( $\beta = 1/2\pi/D$ ) are plotted. The influence of the terms also depends on the magnitude of the derivatives of the envelope functions. Assuming Gaussian incident pulses  $A(0,t) = \exp(-t^2/2T_0^2)$ , these derivatives are proportional to  $1/T_0$  and hence the magnitude of the terms is roughly  $\delta_i/T_0$ . For 10ps pulses,  $T_0 = 10^{-11}$ s and hence the maximum of  $\delta_2/T_0$  will be of the order of  $5 \times 10^{-6} \text{W}^{-1} \text{m}^{-2}$  which is about three orders of magnitude less than the maximum of the SPM coefficient which is  $\gamma_{max} = 6 \times 10^{-3} \text{W}^{-1} \text{m}^{-2}$  for  $\beta = 1/2\pi/D$ . It is therefore reasonable to deduce that the higher order nonlinear terms will not significantly affect the pulse propagation. The value of the higher order nonlinear coefficients near the band edge ( $\beta = 0.05\pi/D$ ) are plotted in Fig. 5. For  $T_0 = 10^{-11}$ s, the maximum of  $\delta_2/T_0$  becomes  $1.4 \times 10^{-3} \text{W}^{-1} \text{m}^{-2}$ , which is now 2 order of magnitude less than  $\gamma_{max} = 1.3 \times 10^{-1} \text{W}^{-1} \text{m}^{-2}$ . This means that the higher order terms have a more pronounced influence near the band edges and for pulse durations less than 10ps, they have to be included in the analysis.

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